# Benzoic acid, 2-ethyl, ethyl ester

**Inchi:** InChI=1S/C11H14O2/c1-3-9-7-5-6-8-10(9)11(12)13-4-2/h5-8H,3-4H2,1-2H3
**InchiKey:** XSXVXSCMWUJXOS-UHFFFAOYSA-N
**Formula:** C11H14O2
**SMILES:** CCOC(=O)c1ccccc1CC
**Mol. weight [g/mol]:** 178.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -89.40 | kJ/mol | Joback Method |
| hf | -290.11 | kJ/mol | Joback Method |
| hfus | 20.69 | kJ/mol | Joback Method |
| hvap | 52.17 | kJ/mol | Joback Method |
| log10ws | -2.94 | | Crippen Method |
| logp | 2.426 | | Crippen Method |
| mcvol | 149.530 | ml/mol | McGowan Method |
| pc | 2735.42 | kPa | Joback Method |
| rinpol | 1272.00 | | NIST Webbook |
| tb | 559.03 | K | Joback Method |
| tc | 769.35 | K | Joback Method |
| tf | 324.83 | K | Joback Method |
| vc | 0.568 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 346.15 | J/mol×K | 559.03 | Joback Method |
| cpg | 360.31 | J/mol×K | 594.08 | Joback Method |
| cpg | 373.70 | J/mol×K | 629.14 | Joback Method |
| cpg | 386.36 | J/mol×K | 664.19 | Joback Method |
| cpg | 398.29 | J/mol×K | 699.24 | Joback Method |
| cpg | 409.50 | J/mol×K | 734.30 | Joback Method |
| cpg | 420.01 | J/mol×K | 769.35 | Joback Method |
| dvisc | 0.0017437 | Pa×s | 324.83 | Joback Method |
| dvisc | 0.0009957 | Pa×s | 363.86 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0006338 | Pa×s | 402.90 | Joback Method |
| dvisc | 0.0004369 | Pa×s | 441.93 | Joback Method |
| dvisc | 0.0003200 | Pa×s | 480.96 | Joback Method |
| dvisc | 0.0002455 | Pa×s | 520.00 | Joback Method |
| dvisc | 0.0001955 | Pa×s | 559.03 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R553505&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**rinpol:** Non-polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume